

Tetraaquabis(3,5-dinitrobenzoato- κO^1)-magnesium tetrahydrate

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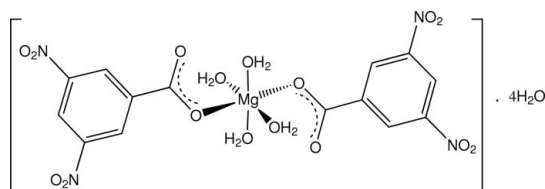
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Key indicators: single-crystal X-ray study; $T = 200$ K; mean $\sigma(C-C) = 0.002$ Å; R factor = 0.036; wR factor = 0.095; data-to-parameter ratio = 13.5.

In the structure of the title compound, $[Mg(C_7H_3N_2O_6)_2 \cdot (H_2O)_4] \cdot 4H_2O$, the slightly distorted octahedral MgO_6 coordination polyhedron comprises two *trans*-related carboxylate O-atom donors from monodentate 3,5-dinitrobenzoate ligands, and four water molecules. The coordinating water molecules and the four water molecules of solvation give both intra- and inter-unit $O-H \cdots O$ hydrogen-bonding interactions with carboxylate, water and nitro O-atom acceptors, forming a three-dimensional structure.

Related literature

For the structures of some magnesium complexes with nitro-substituted benzoic acids, see: Morgant *et al.* (2006); Srinivasan *et al.* (2007, 2011); Arlin *et al.* (2011).



Experimental

Crystal data

$[Mg(C_7H_3N_2O_6)_2(H_2O)_4] \cdot 4H_2O$
 $M_r = 590.67$
Triclinic, $P\bar{1}$
 $a = 7.1748$ (3) Å
 $b = 11.7299$ (6) Å
 $c = 15.0103$ (7) Å
 $\alpha = 103.224$ (4)°
 $\beta = 98.569$ (4)°
 $\gamma = 92.181$ (4)°
 $V = 1212.62$ (10) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.18$ mm⁻¹
 $T = 200$ K
 $0.32 \times 0.22 \times 0.10$ mm

Data collection

Oxford Diffraction Gemini-S CCD-detector diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
 $T_{min} = 0.970$, $T_{max} = 0.980$
15059 measured reflections
4764 independent reflections
3969 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.095$
 $S = 0.94$
4764 reflections
352 parameters
H-atom parameters constrained
 $\Delta\rho_{max} = 0.29$ e Å⁻³
 $\Delta\rho_{min} = -0.20$ e Å⁻³

Table 1

Selected bond lengths (Å).

Mg1—O1W	2.0929 (14)	Mg1—O4W	2.0804 (13)
Mg1—O2W	2.0732 (13)	Mg1—O11A	2.0304 (13)
Mg1—O3W	2.1024 (14)	Mg1—O11B	2.0237 (13)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W—H11W ⁱ ··O8W	0.91	1.79	2.700 (2)	179
O1W—H12W ⁱ ··O6W ⁱ	0.88	1.93	2.7934 (19)	170
O2W—H21W ⁱ ··O12A	0.76	2.11	2.8001 (18)	152
O2W—H22W ⁱ ··O6W	0.87	1.87	2.7375 (18)	178
O3W—H31W ⁱ ··O7W	0.80	2.02	2.8213 (19)	170
O3W—H32W ⁱ ··O5W ⁱⁱ	0.90	1.89	2.7722 (18)	170
O4W—H41W ⁱ ··O12B	0.80	2.00	2.7310 (18)	151
O4W—H42W ⁱ ··O5W ⁱⁱⁱ	0.83	1.97	2.7986 (18)	174
O5W—H51W ⁱ ··O7W ⁱⁱⁱ	0.86	2.11	2.9449 (19)	164
O5W—H52W ⁱ ··O1W	0.86	2.17	2.9702 (19)	155
O6W—H61W ⁱ ··O12A ⁱ	0.86	2.00	2.8404 (19)	163
O6W—H62W ⁱ ··O3W ^{iv}	0.86	2.14	2.9522 (19)	159
O7W—H71W ⁱ ··O12B ^v	0.89	1.87	2.708 (2)	158
O7W—H72W ⁱ ··O32B ^{vi}	0.86	2.50	3.236 (2)	145
O8W—H81W ⁱ ··O12A ⁱ	0.90	1.99	2.7737 (19)	145

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+1, y, z$; (iii) $-x+1, -y, -z+1$; (iv) $-x+2, -y+1, -z+1$; (v) $-x+2, -y, -z+1$; (vi) $x, y, z+1$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) within *WinGX* (Farrugia, 2012); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5305).

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supplementary materials

Acta Cryst. (2013). E69, m215 [doi:10.1107/S160053681300682X]

Tetraaquabis(3,5-dinitrobenzoato- κ O¹)magnesium tetrahydrate

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Comment

Magnesium complexes involving monoanionic nitro-substituted benzoate ligands (*L*) show both the common $[\text{Mg}(\text{H}_2\text{O})_6]^{2+} 2(L)$ form, *e.g.* a dihydrate: *L* = 4-nitrobenzoate (Srinivasan *et al.*, 2007; Arlin *et al.*, 2011), as well as examples in which the ligand is coordinated, *e.g.* $[\text{MgL}(\text{H}_2\text{O})_5] (L)$. HL. H_2O (a complex acid adduct: *L* = 4-nitro-3-hydroxybenzoate) (Morgant *et al.*, 2006) and $[\text{MgL}_2(\text{H}_2\text{O})_4] (L = 2\text{-nitrobenzoate})$ (Srinivasan *et al.*, 2011; Arlin *et al.*, 2011). All known examples are monomeric and have essentially octahedral metal stereochemistry.

The title complex, $[\text{Mg}(\text{C}_7\text{H}_3\text{N}_2\text{O}_6)_2(\text{H}_2\text{O})_4] \cdot 4\text{H}_2\text{O}$ was obtained from the reaction of 3,5-dinitrobenzoic acid with MgCO_3 in aqueous ethanol and the structure is reported here. In this structure (Fig. 1), the slightly distorted octahedral MgO_6 coordination polyhedron comprises two *trans*-related carboxyl O-atom donors from mononodentate 3,5-dinitrobenzoate ligands, and four water molecules [bond range $\text{Mg}-\text{O}$, 2.0237 (13)–2.1024 (14) Å (Table 1)]. The coordinated water molecules and the four water molecules of solvation give both intra- and inter-unit $\text{O}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions with carboxyl, water and nitro O-atom acceptors (Table 2), giving a three-dimensional structure (Fig. 2).

In the present complex, the two 3,5-dinitrobenzoate ligands are conformationally similar, with the carboxyl groups lying essentially in the plane of the benzene ring [torsion angles $\text{C2}-\text{C1}-\text{C11}-\text{O11} = 178.01 (14)^\circ (A)$ and $178.90 (14)^\circ (B)$]. The C5 nitro groups are variously rotated out of the benzene plane [torsion angles $\text{C2}-\text{C3}-\text{N3}-\text{O32} = 154.31 (17)^\circ (A)$ and $159.03 (15)^\circ (B)$; $\text{C4}-\text{C5}-\text{N5}-\text{O52} = 167.74 (15)^\circ (A)$ and $163.06 (15)^\circ (B)$].

Experimental

The title compound was synthesized by the addition of excess MgCO_3 to 15 ml of a hot aqueous ethanolic solution (10:1) of 3,5-dinitrobenzoic acid (0.1 g). After completion of the reaction, the excess MgCO_3 was removed by filtration and the solution was allowed to evaporate to partial dryness at room temperature, giving colourless plates of the title compound from which a specimen was cleaved for the X-ray analysis.

Refinement

Hydrogen atoms on all water molecules were located by difference methods and both positional and isotropic displacement parameters were initially refined but these were then allowed to ride, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. Other H-atoms were included in the refinement at calculated positions [$\text{C}-\text{H} = 0.93$ Å] with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ also using a riding-model approximation.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) within *WinGX* (Farrugia, 2012); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON* (Spek, 2009).

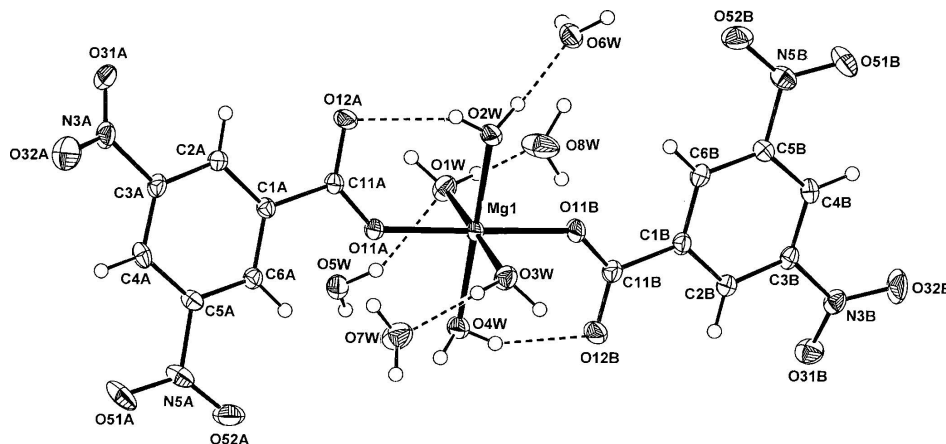


Figure 1

Molecular configuration and atom naming scheme for the title complex, with displacement ellipsoids drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

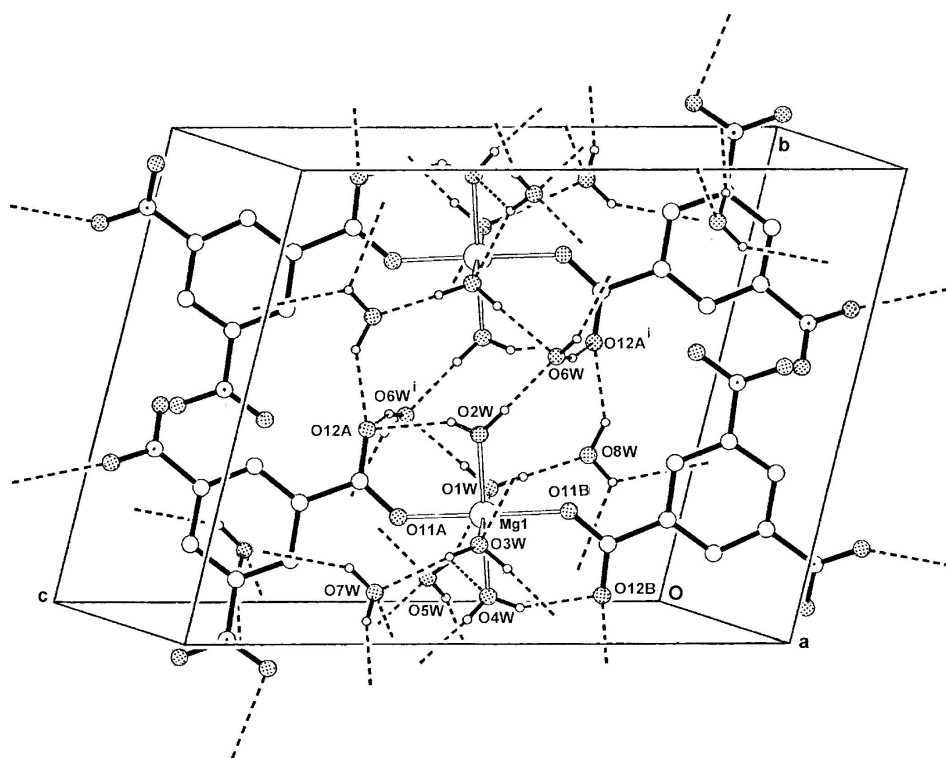


Figure 2

A perspective view of the title complex showing hydrogen-bonding interactions as dashed lines and with non-associative H-atoms omitted. For symmetry code (i), see Table 2.

Tetraaquabis(3,5-dinitrobenzoato- κO^1)magnesium tetrahydrate

Crystal data

$[\text{Mg}(\text{C}_7\text{H}_3\text{N}_2\text{O}_6)_2(\text{H}_2\text{O})_4] \cdot 4\text{H}_2\text{O}$

$M_r = 590.67$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 7.1748\ (3)\ \text{\AA}$

$b = 11.7299\ (6)\ \text{\AA}$

$c = 15.0103 (7) \text{ \AA}$
 $\alpha = 103.224 (4)^\circ$
 $\beta = 98.569 (4)^\circ$
 $\gamma = 92.181 (4)^\circ$
 $V = 1212.62 (10) \text{ \AA}^3$
 $Z = 2$
 $F(000) = 612$
 $D_x = 1.618 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Cell parameters from 4480 reflections
 $\theta = 3.3\text{--}28.8^\circ$
 $\mu = 0.18 \text{ mm}^{-1}$
 $T = 200 \text{ K}$
Plate, colourless
 $0.32 \times 0.22 \times 0.10 \text{ mm}$

Data collection

Oxford Diffraction Gemini-S CCD-detector
diffractometer
Radiation source: Enhance(Mo) X-ray source
Graphite monochromator
Detector resolution: $16.077 \text{ pixels mm}^{-1}$
 ω scans
Absorption correction: multi-scan
(*Crys.Alis PRO*; Agilent, 2012)
 $T_{\min} = 0.970$, $T_{\max} = 0.980$

15059 measured reflections
4764 independent reflections
3969 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 $\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 3.3^\circ$
 $h = -8 \rightarrow 8$
 $k = -14 \rightarrow 14$
 $l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.095$
 $S = 0.94$
4764 reflections
352 parameters
0 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.5437P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.29 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.20 \text{ e \AA}^{-3}$

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Mg1	0.72688 (8)	0.24686 (5)	0.49442 (4)	0.0206 (2)
O1W	0.45776 (18)	0.27809 (11)	0.43347 (9)	0.0315 (4)
O2W	0.80173 (18)	0.42361 (10)	0.55275 (8)	0.0287 (4)
O3W	0.99516 (17)	0.20820 (11)	0.55261 (9)	0.0289 (4)
O4W	0.65142 (18)	0.06937 (10)	0.43663 (8)	0.0283 (4)
O11A	0.62746 (18)	0.23370 (10)	0.61171 (8)	0.0255 (4)
O11B	0.83217 (18)	0.26394 (10)	0.37996 (8)	0.0278 (4)
O12A	0.5701 (2)	0.41362 (10)	0.68573 (9)	0.0318 (4)
O12B	0.8071 (2)	0.08551 (11)	0.28425 (9)	0.0325 (4)
O31A	0.31477 (19)	0.44416 (11)	0.97944 (9)	0.0340 (4)

O31B	0.8787 (2)	0.06471 (11)	−0.04095 (9)	0.0351 (4)
O32A	0.4359 (3)	0.33267 (14)	1.06560 (10)	0.0526 (6)
O32B	1.0519 (2)	0.20264 (14)	−0.06886 (10)	0.0476 (5)
O51A	0.5101 (2)	−0.07040 (12)	0.88966 (10)	0.0432 (5)
O51B	1.0734 (2)	0.59134 (12)	0.13968 (10)	0.0420 (5)
O52A	0.6406 (2)	−0.08279 (12)	0.76731 (10)	0.0429 (5)
O52B	0.9300 (2)	0.60972 (12)	0.25868 (10)	0.0447 (5)
N3A	0.3977 (2)	0.35844 (14)	0.99081 (10)	0.0303 (5)
N3B	0.9615 (2)	0.16217 (13)	−0.01841 (10)	0.0273 (5)
N5A	0.5629 (2)	−0.02866 (13)	0.82933 (11)	0.0300 (5)
N5B	0.9901 (2)	0.55022 (13)	0.19201 (11)	0.0288 (5)
C1A	0.5416 (2)	0.25645 (14)	0.75959 (11)	0.0191 (5)
C1B	0.8897 (2)	0.25074 (15)	0.22763 (11)	0.0221 (5)
C2A	0.4858 (2)	0.32878 (14)	0.83639 (11)	0.0215 (5)
C2B	0.9050 (2)	0.18121 (15)	0.14109 (11)	0.0229 (5)
C3A	0.4564 (2)	0.28082 (15)	0.90967 (11)	0.0235 (5)
C3B	0.9496 (2)	0.23575 (15)	0.07369 (11)	0.0227 (5)
C4A	0.4796 (2)	0.16471 (15)	0.91068 (12)	0.0255 (5)
C4B	0.9805 (2)	0.35601 (15)	0.08781 (12)	0.0245 (5)
C5A	0.5332 (2)	0.09582 (14)	0.83218 (12)	0.0226 (5)
C5B	0.9603 (2)	0.42181 (15)	0.17419 (12)	0.0228 (5)
C6A	0.5640 (2)	0.13877 (14)	0.75691 (11)	0.0211 (5)
C6B	0.9152 (2)	0.37241 (15)	0.24432 (11)	0.0227 (5)
C11A	0.5832 (2)	0.30567 (14)	0.67950 (11)	0.0211 (5)
C11B	0.8402 (2)	0.19519 (15)	0.30354 (12)	0.0234 (5)
O5W	0.21801 (18)	0.07011 (11)	0.44221 (9)	0.0295 (4)
O6W	0.75569 (18)	0.58555 (11)	0.44724 (9)	0.0298 (4)
O7W	1.0086 (2)	0.11013 (12)	0.70823 (9)	0.0413 (5)
O8W	0.4051 (3)	0.34282 (12)	0.27062 (10)	0.0526 (6)
H2A	0.46860	0.40750	0.83860	0.0260*
H2B	0.88570	0.09990	0.12880	0.0270*
H4A	0.46040	0.13470	0.96110	0.0310*
H4B	1.01310	0.39060	0.04180	0.0290*
H6A	0.59920	0.08960	0.70520	0.0250*
H6B	0.90230	0.41970	0.30160	0.0270*
H11W	0.43930	0.30080	0.37910	0.0470*
H12W	0.37960	0.31880	0.46530	0.0470*
H21W	0.73890	0.44440	0.58890	0.0430*
H22W	0.79040	0.47460	0.51890	0.0430*
H31W	1.01100	0.18470	0.59930	0.0430*
H32W	1.05640	0.16380	0.51110	0.0430*
H41W	0.69830	0.04970	0.39120	0.0420*
H42W	0.68820	0.02370	0.46960	0.0420*
H51W	0.16520	0.02280	0.39150	0.0440*
H52W	0.30810	0.11320	0.43140	0.0440*
H61W	0.66770	0.57420	0.39940	0.0450*
H62W	0.84670	0.63140	0.44130	0.0450*
H71W	1.07840	0.05610	0.72630	0.0620*
H72W	1.00000	0.16100	0.75820	0.0620*

H81W	0.42210	0.41470	0.26020	0.0790*
H82W	0.40670	0.28650	0.22020	0.0790*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0281 (3)	0.0207 (3)	0.0153 (3)	0.0025 (2)	0.0077 (2)	0.0060 (2)
O1W	0.0356 (7)	0.0391 (8)	0.0244 (7)	0.0139 (6)	0.0088 (5)	0.0129 (6)
O2W	0.0430 (8)	0.0220 (6)	0.0251 (7)	0.0031 (5)	0.0129 (6)	0.0089 (5)
O3W	0.0328 (7)	0.0321 (7)	0.0250 (7)	0.0092 (5)	0.0088 (5)	0.0097 (6)
O4W	0.0399 (7)	0.0237 (6)	0.0228 (6)	0.0013 (5)	0.0099 (5)	0.0059 (5)
O11A	0.0404 (7)	0.0216 (6)	0.0179 (6)	0.0038 (5)	0.0136 (5)	0.0056 (5)
O11B	0.0415 (7)	0.0256 (6)	0.0190 (6)	0.0001 (5)	0.0136 (5)	0.0055 (5)
O12A	0.0574 (9)	0.0193 (6)	0.0236 (7)	0.0065 (6)	0.0152 (6)	0.0088 (5)
O12B	0.0526 (8)	0.0236 (7)	0.0247 (7)	0.0023 (6)	0.0136 (6)	0.0078 (5)
O31A	0.0372 (7)	0.0306 (7)	0.0344 (8)	0.0046 (6)	0.0177 (6)	0.0003 (6)
O31B	0.0460 (8)	0.0303 (7)	0.0251 (7)	0.0022 (6)	0.0021 (6)	0.0010 (6)
O32A	0.0864 (12)	0.0571 (10)	0.0185 (7)	0.0109 (9)	0.0189 (7)	0.0099 (7)
O32B	0.0645 (10)	0.0541 (10)	0.0262 (8)	−0.0070 (8)	0.0260 (7)	0.0035 (7)
O51A	0.0639 (10)	0.0333 (8)	0.0357 (8)	−0.0119 (7)	0.0008 (7)	0.0221 (7)
O51B	0.0491 (9)	0.0371 (8)	0.0434 (9)	−0.0119 (7)	0.0087 (7)	0.0187 (7)
O52A	0.0676 (10)	0.0223 (7)	0.0389 (8)	0.0090 (7)	0.0113 (7)	0.0047 (6)
O52B	0.0724 (11)	0.0252 (7)	0.0356 (8)	0.0060 (7)	0.0147 (7)	0.0014 (6)
N3A	0.0367 (9)	0.0340 (9)	0.0208 (8)	−0.0016 (7)	0.0129 (7)	0.0034 (7)
N3B	0.0321 (8)	0.0322 (9)	0.0179 (7)	0.0062 (7)	0.0059 (6)	0.0048 (7)
N5A	0.0414 (9)	0.0209 (8)	0.0271 (8)	−0.0037 (7)	−0.0023 (7)	0.0104 (7)
N5B	0.0337 (8)	0.0254 (8)	0.0264 (8)	−0.0017 (6)	−0.0012 (7)	0.0090 (7)
C1A	0.0215 (8)	0.0205 (8)	0.0159 (8)	0.0001 (6)	0.0035 (6)	0.0054 (7)
C1B	0.0234 (8)	0.0258 (9)	0.0193 (8)	0.0033 (7)	0.0076 (7)	0.0067 (7)
C2A	0.0260 (9)	0.0204 (8)	0.0188 (8)	0.0029 (7)	0.0053 (7)	0.0051 (7)
C2B	0.0267 (9)	0.0227 (9)	0.0203 (9)	0.0021 (7)	0.0073 (7)	0.0048 (7)
C3A	0.0269 (9)	0.0278 (9)	0.0160 (8)	0.0013 (7)	0.0077 (7)	0.0033 (7)
C3B	0.0242 (9)	0.0284 (9)	0.0160 (8)	0.0041 (7)	0.0064 (7)	0.0042 (7)
C4A	0.0298 (9)	0.0313 (10)	0.0178 (8)	−0.0032 (7)	0.0047 (7)	0.0114 (7)
C4B	0.0254 (9)	0.0307 (9)	0.0204 (9)	0.0003 (7)	0.0069 (7)	0.0102 (8)
C5A	0.0278 (9)	0.0187 (8)	0.0214 (9)	−0.0011 (7)	0.0017 (7)	0.0067 (7)
C5B	0.0237 (8)	0.0226 (9)	0.0225 (9)	0.0005 (7)	0.0031 (7)	0.0071 (7)
C6A	0.0242 (8)	0.0216 (8)	0.0173 (8)	0.0006 (7)	0.0051 (7)	0.0034 (7)
C6B	0.0247 (9)	0.0265 (9)	0.0167 (8)	0.0024 (7)	0.0055 (7)	0.0034 (7)
C11A	0.0265 (9)	0.0220 (9)	0.0160 (8)	0.0018 (7)	0.0054 (7)	0.0057 (7)
C11B	0.0266 (9)	0.0254 (9)	0.0198 (9)	0.0039 (7)	0.0072 (7)	0.0061 (7)
O5W	0.0327 (7)	0.0281 (7)	0.0284 (7)	−0.0004 (5)	0.0101 (5)	0.0053 (6)
O6W	0.0316 (7)	0.0293 (7)	0.0319 (7)	0.0014 (5)	0.0073 (6)	0.0130 (6)
O7W	0.0530 (9)	0.0423 (8)	0.0308 (8)	0.0173 (7)	0.0087 (7)	0.0097 (7)
O8W	0.1022 (14)	0.0273 (8)	0.0264 (8)	0.0089 (8)	0.0032 (8)	0.0064 (6)

Geometric parameters (\AA , $^\circ$)

Mg1—O1W	2.0929 (14)	O6W—H62W	0.8600
Mg1—O2W	2.0732 (13)	O7W—H72W	0.8600

Mg1—O3W	2.1024 (14)	O7W—H71W	0.8900
Mg1—O4W	2.0804 (13)	O8W—H81W	0.9000
Mg1—O11A	2.0304 (13)	O8W—H82W	0.8900
Mg1—O11B	2.0237 (13)	N3A—C3A	1.471 (2)
O11A—C11A	1.254 (2)	N3B—C3B	1.469 (2)
O11B—C11B	1.253 (2)	N5A—C5A	1.476 (2)
O12A—C11A	1.256 (2)	N5B—C5B	1.470 (2)
O12B—C11B	1.258 (2)	C1A—C2A	1.387 (2)
O31A—N3A	1.220 (2)	C1A—C6A	1.388 (2)
O31B—N3B	1.219 (2)	C1A—C11A	1.510 (2)
O32A—N3A	1.223 (2)	C1B—C6B	1.391 (3)
O32B—N3B	1.228 (2)	C1B—C11B	1.514 (2)
O51A—N5A	1.222 (2)	C1B—C2B	1.389 (2)
O51B—N5B	1.224 (2)	C2A—C3A	1.384 (2)
O52A—N5A	1.221 (2)	C2B—C3B	1.383 (2)
O52B—N5B	1.227 (2)	C3A—C4A	1.382 (3)
O1W—H11W	0.9100	C3B—C4B	1.382 (3)
O1W—H12W	0.8800	C4A—C5A	1.383 (2)
O2W—H21W	0.7600	C4B—C5B	1.380 (2)
O2W—H22W	0.8700	C5A—C6A	1.380 (2)
O3W—H32W	0.9000	C5B—C6B	1.384 (2)
O3W—H31W	0.8000	C2A—H2A	0.9300
O4W—H41W	0.8000	C2B—H2B	0.9300
O4W—H42W	0.8300	C4A—H4A	0.9300
O5W—H51W	0.8600	C4B—H4B	0.9300
O5W—H52W	0.8600	C6A—H6A	0.9300
O6W—H61W	0.8600	C6B—H6B	0.9300
Mg1…H52W	3.2400	O12B…H2B	2.5200
Mg1…H62W ⁱ	3.2400	O12B…H41W	2.0000
O1W…O2W	3.0289 (18)	O12B…H71W ^{vi}	1.8700
O1W…O4W	2.8669 (18)	O31A…H4B ^x	2.5900
O1W…O5W	2.9702 (19)	O31A…H2A	2.4900
O1W…O8W	2.700 (2)	O31B…H2B	2.4800
O1W…O11A	2.9371 (18)	O31B…H2B ^{xi}	2.8400
O1W…O11B	2.9163 (18)	O32A…H81W ^{vii}	2.8800
O1W…O6W ⁱⁱ	2.7934 (19)	O32A…H4A	2.5200
O2W…O12A	2.8001 (18)	O32A…H82W ^{vii}	2.5400
O2W…O1W	3.0289 (18)	O32B…H4B	2.4900
O2W…O3W	2.9285 (18)	O32B…H72W ^{viii}	2.5000
O2W…O6W	2.7375 (18)	O51A…H82W ^{iv}	2.8300
O2W…O11A	2.8859 (17)	O51A…H4A ^{xiv}	2.5100
O2W…O11B	2.8740 (17)	O51A…H2B ^{iv}	2.8100
O2W…C11A	3.150 (2)	O51A…H4A	2.4600
O2W…O6W ⁱ	3.1813 (19)	O51B…H4B	2.4600
O3W…O11A	2.9108 (18)	O51B…H4B ^{xii}	2.7600
O3W…O6W ⁱ	2.9522 (19)	O52A…H82W ^{iv}	2.4500
O3W…O2W	2.9285 (18)	O52A…H6A	2.4200
O3W…O4W	2.9804 (18)	O52B…H62W	2.8500

O3W...O5W ⁱⁱⁱ	2.7722 (18)	O52B...H6B	2.4700
O3W...O7W	2.8213 (19)	O52B...H31W ⁱ	2.8000
O3W...O52B ⁱ	3.093 (2)	O52B...H72W ⁱ	2.7900
O3W...O11B	2.9054 (18)	N3A...O31A ^{ix}	2.951 (2)
O4W...O12B	2.7310 (18)	N3A...O32B ^x	2.923 (2)
O4W...O5W	3.1235 (19)	N3B...O31B ^{xi}	3.194 (2)
O4W...C11B	3.163 (2)	N5A...O12B ^{iv}	2.897 (2)
O4W...O1W	2.8669 (18)	N5A...O31B ^{vii}	2.765 (2)
O4W...O3W	2.9804 (18)	N5B...O31A ⁱⁱ	3.134 (2)
O4W...O5W ^{iv}	2.7986 (18)	C1A...O51B ⁱ	3.201 (2)
O4W...O11A	2.9144 (17)	C2A...O52B ⁱⁱ	3.290 (2)
O4W...O11B	2.9336 (17)	C2A...O51B ⁱ	3.208 (2)
O5W...O1W	2.9702 (19)	C2B...O51A ^{iv}	3.130 (2)
O5W...O4W	3.1235 (19)	C3A...O32B ^x	3.095 (2)
O5W...O7W ^{iv}	2.9449 (19)	C4A...O32B ^x	3.167 (2)
O5W...O4W ^{iv}	2.7986 (18)	C4A...O51A ^{xiv}	3.416 (2)
O5W...O3W ^v	2.7722 (18)	C4A...O31B ^{vii}	3.183 (2)
O6W...O12A ⁱⁱ	2.8404 (19)	C4B...O32A ^{xiii}	3.349 (3)
O6W...O2W ⁱ	3.1813 (19)	C4B...O31A ^{xiii}	3.348 (2)
O6W...O3W ⁱ	2.9522 (19)	C5A...O12B ^{iv}	3.189 (2)
O6W...O2W	2.7375 (18)	C5A...O31B ^{vii}	2.981 (2)
O6W...C11A ⁱⁱ	3.336 (2)	C6A...O7W	3.389 (2)
O6W...O1W ⁱⁱ	2.7934 (19)	C11A...O6W ⁱⁱ	3.336 (2)
O7W...O52B ⁱ	3.212 (2)	C11A...O51B ⁱ	3.343 (2)
O7W...C6A	3.389 (2)	C6A...H41W ^{iv}	3.0900
O7W...O5W ^{iv}	2.9449 (19)	C11A...H61W ⁱⁱ	2.6400
O7W...O3W	2.8213 (19)	C11A...H21W	2.6600
O7W...O12B ^{vi}	2.708 (2)	C11B...H41W	2.6400
O7W...O32B ^{vii}	3.236 (2)	C11B...H71W ^{vi}	2.9700
O8W...O12A ⁱⁱ	2.7737 (19)	H2A...O31A	2.4900
O8W...O52A ^{iv}	2.968 (2)	H2A...O12A	2.5200
O8W...O32A ^{viii}	3.094 (2)	H2B...O51A ^{iv}	2.8100
O8W...O1W	2.700 (2)	H2B...O12B	2.5200
O11A...O1W	2.9371 (18)	H2B...O31B	2.4800
O11A...O3W	2.9108 (18)	H2B...O31B ^{xi}	2.8400
O11A...O4W	2.9144 (17)	H4A...O51A ^{xiv}	2.5100
O11A...O2W	2.8859 (17)	H4A...O32A	2.5200
O11B...O3W	2.9054 (18)	H4A...O51A	2.4600
O11B...O2W	2.8740 (17)	H4B...O31A ^{xiii}	2.5900
O11B...O4W	2.9336 (17)	H4B...O51B ^{xii}	2.7600
O11B...O1W	2.9163 (18)	H4B...O32B	2.4900
O12A...O6W ⁱⁱ	2.8404 (19)	H4B...O51B	2.4600
O12A...O2W	2.8001 (18)	H6A...O52A	2.4200
O12A...O8W ⁱⁱ	2.7737 (19)	H6A...H51W ^{iv}	2.5900
O12B...N5A ^{iv}	2.897 (2)	H6A...O11A	2.4500
O12B...O51A ^{iv}	3.164 (2)	H6A...O4W ^{iv}	2.8300
O12B...C5A ^{iv}	3.189 (2)	H6B...O52B	2.4700
O12B...O7W ^{vi}	2.708 (2)	H6B...O11B	2.4600
O12B...O52A ^{iv}	3.187 (2)	H11W...O8W	1.7900

O12B...O4W	2.7310 (18)	H11W...H82W	2.3300
O31A...N3A ^{ix}	2.951 (2)	H11W...H81W	2.4500
O31A...O32B ^x	3.218 (2)	H12W...H52W	2.3700
O31A...C4B ^x	3.348 (2)	H12W...H62W ⁱⁱ	2.3100
O31A...O31A ^{ix}	2.8352 (19)	H12W...O6W ⁱⁱ	1.9300
O31A...N5B ⁱⁱ	3.134 (2)	H12W...H61W ⁱⁱ	2.2100
O31A...O51B ⁱⁱ	3.036 (2)	H21W...O12A	2.1100
O31B...O31B ^{xi}	2.6950 (19)	H21W...C11A	2.6600
O31B...C5A ^{viii}	2.981 (2)	H22W...H61W	2.4300
O31B...O51A ^{viii}	2.949 (2)	H22W...H62W	2.4400
O31B...N5A ^{viii}	2.765 (2)	H22W...O6W	1.8700
O31B...O52A ^{viii}	3.198 (2)	H31W...O52B ⁱ	2.8000
O31B...N3B ^{xi}	3.194 (2)	H31W...H72W	2.4800
O31B...C4A ^{viii}	3.183 (2)	H31W...O7W	2.0200
O32A...C4B ^x	3.349 (3)	H31W...H62W ⁱ	2.5900
O32A...O8W ^{vii}	3.094 (2)	H32W...H52W ⁱⁱⁱ	2.3300
O32B...O51B ^{xii}	2.972 (2)	H32W...H51W ⁱⁱⁱ	2.3900
O32B...N3A ^{xiii}	2.923 (2)	H32W...H62W ⁱ	2.3900
O32B...O7W ^{viii}	3.236 (2)	H32W...O5W ⁱⁱⁱ	1.8900
O32B...O31A ^{xiii}	3.218 (2)	H41W...O12B	2.0000
O32B...C4A ^{xiii}	3.167 (2)	H41W...C11B	2.6400
O32B...C3A ^{xiii}	3.095 (2)	H41W...C6A ^{iv}	3.0900
O51A...O12B ^{iv}	3.164 (2)	H42W...H52W ^{iv}	2.4200
O51A...C2B ^{iv}	3.130 (2)	H42W...O5W ^{iv}	1.9700
O51A...C4A ^{xiv}	3.416 (2)	H42W...H51W ^{iv}	2.3800
O51A...O31B ^{vii}	2.949 (2)	H51W...H42W ^{iv}	2.3800
O51B...O31A ⁱⁱ	3.036 (2)	H51W...O7W ^{iv}	2.1100
O51B...O32B ^{xii}	2.972 (2)	H51W...H71W ^{iv}	2.2900
O51B...C11A ⁱ	3.343 (2)	H51W...H6A ^{iv}	2.5900
O51B...C2A ⁱ	3.208 (2)	H51W...H32W ^v	2.3900
O51B...C1A ⁱ	3.201 (2)	H52W...H12W	2.3700
O52A...O8W ^{iv}	2.968 (2)	H52W...Mg1	3.2400
O52A...O12B ^{iv}	3.187 (2)	H52W...O1W	2.1700
O52A...O31B ^{vii}	3.198 (2)	H52W...H32W ^v	2.3300
O52B...C2A ⁱⁱ	3.290 (2)	H52W...H42W ^{iv}	2.4200
O52B...O3W ⁱ	3.093 (2)	H52W...O4W	2.5300
O52B...O7W ⁱ	3.212 (2)	H61W...O12A ⁱⁱ	2.0000
O1W...H52W	2.1700	H61W...C11A ⁱⁱ	2.6400
O2W...H62W ⁱ	2.6200	H61W...H12W ⁱⁱ	2.2100
O3W...H62W ⁱ	2.1400	H61W...H22W	2.4300
O4W...H6A ^{iv}	2.8300	H62W...H31W ⁱ	2.5900
O4W...H52W	2.5300	H62W...H22W	2.4400
O5W...H42W ^{iv}	1.9700	H62W...O52B	2.8500
O5W...H32W ^v	1.8900	H62W...Mg1 ⁱ	3.2400
O6W...H12W ⁱⁱ	1.9300	H62W...O2W ⁱ	2.6200
O6W...H22W	1.8700	H62W...O3W ⁱ	2.1400
O7W...H31W	2.0200	H62W...H12W ⁱⁱ	2.3100
O7W...H51W ^{iv}	2.1100	H62W...H32W ⁱ	2.3900
O8W...H11W	1.7900	H71W...O12B ^{vi}	1.8700

O11A...H21W	2.6800	H71W...C11B ^{vi}	2.9700
O11A...H31W	2.8600	H71W...H51W ^{iv}	2.2900
O11A...H6A	2.4500	H72W...H31W	2.4800
O11B...H41W	2.7100	H72W...O52B ⁱ	2.7900
O11B...H22W	2.9000	H72W...O32B ^{vii}	2.5000
O11B...H32W	2.8500	H81W...O32A ^{viii}	2.8800
O11B...H6B	2.4600	H81W...H11W	2.4500
O11B...H11W	2.8700	H81W...O12A ⁱⁱ	1.9900
O12A...H21W	2.1100	H82W...O32A ^{viii}	2.5400
O12A...H61W ⁱⁱ	2.0000	H82W...H11W	2.3300
O12A...H2A	2.5200	H82W...O51A ^{iv}	2.8300
O12A...H81W ⁱⁱ	1.9900	H82W...O52A ^{iv}	2.4500
O1W—Mg1—O2W	93.28 (6)	O51B—N5B—O52B	123.98 (16)
O1W—Mg1—O3W	177.64 (6)	C6A—C1A—C11A	119.51 (14)
O1W—Mg1—O4W	86.78 (6)	C2A—C1A—C6A	120.12 (15)
O1W—Mg1—O11A	90.83 (6)	C2A—C1A—C11A	120.35 (15)
O1W—Mg1—O11B	90.20 (6)	C2B—C1B—C11B	120.41 (16)
O2W—Mg1—O3W	89.06 (6)	C6B—C1B—C11B	119.53 (14)
O2W—Mg1—O4W	179.66 (6)	C2B—C1B—C6B	120.04 (15)
O2W—Mg1—O11A	89.38 (5)	C1A—C2A—C3A	118.30 (15)
O2W—Mg1—O11B	89.09 (5)	C1B—C2B—C3B	118.44 (16)
O3W—Mg1—O4W	90.88 (6)	N3A—C3A—C4A	118.58 (15)
O3W—Mg1—O11A	89.53 (6)	N3A—C3A—C2A	117.81 (15)
O3W—Mg1—O11B	89.50 (6)	C2A—C3A—C4A	123.62 (15)
O4W—Mg1—O11A	90.29 (5)	N3B—C3B—C2B	118.31 (15)
O4W—Mg1—O11B	91.24 (5)	N3B—C3B—C4B	118.16 (15)
O11A—Mg1—O11B	178.20 (6)	C2B—C3B—C4B	123.52 (15)
Mg1—O11A—C11A	134.86 (11)	C3A—C4A—C5A	115.94 (16)
Mg1—O11B—C11B	133.81 (12)	C3B—C4B—C5B	116.09 (16)
H11W—O1W—H12W	103.00	C4A—C5A—C6A	122.98 (16)
Mg1—O1W—H11W	121.00	N5A—C5A—C4A	118.66 (15)
Mg1—O1W—H12W	122.00	N5A—C5A—C6A	118.35 (15)
Mg1—O2W—H22W	121.00	N5B—C5B—C6B	118.97 (15)
H21W—O2W—H22W	104.00	C4B—C5B—C6B	123.07 (17)
Mg1—O2W—H21W	108.00	N5B—C5B—C4B	117.96 (15)
Mg1—O3W—H31W	122.00	C1A—C6A—C5A	119.03 (15)
Mg1—O3W—H32W	113.00	C1B—C6B—C5B	118.81 (15)
H31W—O3W—H32W	108.00	O11A—C11A—O12A	125.65 (15)
Mg1—O4W—H41W	109.00	O11A—C11A—C1A	116.26 (15)
Mg1—O4W—H42W	116.00	O12A—C11A—C1A	118.09 (14)
H41W—O4W—H42W	105.00	O12B—C11B—C1B	117.76 (15)
H51W—O5W—H52W	110.00	O11B—C11B—O12B	125.84 (16)
H61W—O6W—H62W	110.00	O11B—C11B—C1B	116.38 (15)
H71W—O7W—H72W	105.00	C3A—C2A—H2A	121.00
H81W—O8W—H82W	112.00	C1A—C2A—H2A	121.00
O32A—N3A—C3A	117.58 (16)	C3B—C2B—H2B	121.00
O31A—N3A—O32A	124.23 (16)	C1B—C2B—H2B	121.00
O31A—N3A—C3A	118.19 (14)	C3A—C4A—H4A	122.00

O31B—N3B—C3B	118.03 (14)	C5A—C4A—H4A	122.00
O32B—N3B—C3B	118.34 (15)	C3B—C4B—H4B	122.00
O31B—N3B—O32B	123.62 (15)	C5B—C4B—H4B	122.00
O51A—N5A—C5A	117.93 (15)	C5A—C6A—H6A	120.00
O52A—N5A—C5A	117.70 (15)	C1A—C6A—H6A	120.00
O51A—N5A—O52A	124.36 (16)	C1B—C6B—H6B	121.00
O52B—N5B—C5B	117.88 (15)	C5B—C6B—H6B	121.00
O51B—N5B—C5B	118.14 (15)		
O1W—Mg1—O11A—C11A	−76.77 (16)	C11A—C1A—C6A—C5A	177.32 (14)
O2W—Mg1—O11A—C11A	16.50 (16)	C6A—C1A—C11A—O11A	3.6 (2)
O3W—Mg1—O11A—C11A	105.57 (16)	C2A—C1A—C11A—O12A	1.7 (2)
O4W—Mg1—O11A—C11A	−163.55 (16)	C2A—C1A—C6A—C5A	−1.1 (2)
O1W—Mg1—O11B—C11B	−84.11 (16)	C11A—C1A—C2A—C3A	−177.50 (14)
O2W—Mg1—O11B—C11B	−177.38 (16)	C6A—C1A—C2A—C3A	0.9 (2)
O3W—Mg1—O11B—C11B	93.55 (16)	C2B—C1B—C6B—C5B	−1.6 (2)
O4W—Mg1—O11B—C11B	2.68 (16)	C6B—C1B—C2B—C3B	1.3 (2)
Mg1—O11A—C11A—O12A	9.1 (3)	C11B—C1B—C2B—C3B	179.69 (14)
Mg1—O11A—C11A—C1A	−171.22 (11)	C6B—C1B—C11B—O11B	−2.7 (2)
Mg1—O11B—C11B—O12B	−12.6 (3)	C2B—C1B—C11B—O12B	−2.6 (2)
Mg1—O11B—C11B—C1B	165.81 (11)	C11B—C1B—C6B—C5B	−179.97 (13)
O31A—N3A—C3A—C4A	−154.62 (15)	C6B—C1B—C11B—O12B	175.83 (15)
O32A—N3A—C3A—C4A	25.5 (2)	C2B—C1B—C11B—O11B	178.90 (14)
O31A—N3A—C3A—C2A	25.5 (2)	C1A—C2A—C3A—N3A	179.86 (14)
O32A—N3A—C3A—C2A	−154.31 (17)	C1A—C2A—C3A—C4A	0.0 (2)
O31B—N3B—C3B—C2B	21.9 (2)	C1B—C2B—C3B—N3B	−178.65 (13)
O32B—N3B—C3B—C2B	−159.03 (15)	C1B—C2B—C3B—C4B	0.2 (2)
O32B—N3B—C3B—C4B	22.0 (2)	C2A—C3A—C4A—C5A	−0.7 (2)
O31B—N3B—C3B—C4B	−156.99 (15)	N3A—C3A—C4A—C5A	179.43 (14)
O52A—N5A—C5A—C6A	11.0 (2)	N3B—C3B—C4B—C5B	177.46 (13)
O51A—N5A—C5A—C6A	−169.81 (15)	C2B—C3B—C4B—C5B	−1.4 (2)
O52A—N5A—C5A—C4A	−167.74 (15)	C3A—C4A—C5A—C6A	0.5 (2)
O51A—N5A—C5A—C4A	11.5 (2)	C3A—C4A—C5A—N5A	179.18 (14)
O52B—N5B—C5B—C6B	−17.5 (2)	C3B—C4B—C5B—N5B	−179.44 (13)
O51B—N5B—C5B—C6B	162.42 (15)	C3B—C4B—C5B—C6B	1.1 (2)
O51B—N5B—C5B—C4B	−17.0 (2)	N5A—C5A—C6A—C1A	−178.28 (14)
O52B—N5B—C5B—C4B	163.06 (15)	C4A—C5A—C6A—C1A	0.4 (2)
C6A—C1A—C11A—O12A	−176.77 (15)	N5B—C5B—C6B—C1B	−179.11 (14)
C2A—C1A—C11A—O11A	−178.01 (14)	C4B—C5B—C6B—C1B	0.3 (2)

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$; (iii) $x+1, y, z$; (iv) $-x+1, -y, -z+1$; (v) $x-1, y, z$; (vi) $-x+2, -y, -z+1$; (vii) $x, y, z+1$; (viii) $x, y, z-1$; (ix) $-x+1, -y+1, -z+2$; (x) $x-1, y, z+1$; (xi) $-x+2, -y, -z$; (xii) $-x+2, -y+1, -z$; (xiii) $x+1, y, z-1$; (xiv) $-x+1, -y, -z+2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H11W \cdots O8W	0.91	1.79	2.700 (2)	179
O1W—H12W \cdots O6W ⁱⁱ	0.88	1.93	2.7934 (19)	170
O2W—H21W \cdots O12A	0.76	2.11	2.8001 (18)	152
O2W—H22W \cdots O6W	0.87	1.87	2.7375 (18)	178

O3 <i>W</i> —H31 <i>W</i> ...O7 <i>W</i>	0.80	2.02	2.8213 (19)	170
O3 <i>W</i> —H32 <i>W</i> ...O5 <i>W</i> ⁱⁱⁱ	0.90	1.89	2.7722 (18)	170
O4 <i>W</i> —H41 <i>W</i> ...O12 <i>B</i>	0.80	2.00	2.7310 (18)	151
O4 <i>W</i> —H42 <i>W</i> ...O5 <i>W</i> ^{iv}	0.83	1.97	2.7986 (18)	174
O5 <i>W</i> —H51 <i>W</i> ...O7 <i>W</i> ^{iv}	0.86	2.11	2.9449 (19)	164
O5 <i>W</i> —H52 <i>W</i> ...O1 <i>W</i>	0.86	2.17	2.9702 (19)	155
O5 <i>W</i> —H52 <i>W</i> ...O4 <i>W</i>	0.86	2.53	3.1235 (19)	127
O6 <i>W</i> —H61 <i>W</i> ...O12 <i>A</i> ⁱⁱ	0.86	2.00	2.8404 (19)	163
O6 <i>W</i> —H62 <i>W</i> ...O3 <i>W</i> ⁱⁱ	0.86	2.14	2.9522 (19)	159
O7 <i>W</i> —H71 <i>W</i> ...O12 <i>B</i> ^{vi}	0.89	1.87	2.708 (2)	158
O7 <i>W</i> —H72 <i>W</i> ...O32 <i>B</i> ^{vii}	0.86	2.50	3.236 (2)	145
O8 <i>W</i> —H81 <i>W</i> ...O12 <i>A</i> ⁱⁱ	0.90	1.99	2.7737 (19)	145
O8 <i>W</i> —H82 <i>W</i> ...O32 <i>A</i> ^{viii}	0.89	2.54	3.094 (2)	122
O8 <i>W</i> —H82 <i>W</i> ...O52 <i>A</i> ^{iv}	0.89	2.45	2.968 (2)	117
C4 <i>A</i> —H4 <i>A</i> ...O51 <i>A</i> ^{xiv}	0.93	2.51	3.416 (2)	166
C4 <i>B</i> —H4 <i>B</i> ...O31 <i>A</i> ^{xiii}	0.93	2.59	3.348 (2)	139

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